Feynman Integrals with Absorbing Boundaries

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We propose a formulation of an absorbing boundary for a quantum particle. The formulation is based on a Feynman-type integral over trajectories that are confined to the non-absorbing region. Trajectories that reach the absorbing wall are discounted from the population of the surviving trajectories with a certain weighting factor. Under the assumption that absorbed trajectories do not interfere with the surviving trajectories, we obtain a time dependent absorption law. Two examples are worked out.

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The purpose of this letter is to propose a Feynman-type integral to describe absorption of particles in a surface bounding a domain. The need for such description arises for example in scattering theory, in the description of a photographic plate, in the double slit experiment, in neutron optics, and so on. The optical model [1,2] is often used to describe absorption in quantum systems. This model is based on analogy with electro-magnetic wave theory. It is not obvious that the methods of describing absorption in Maxwell's equations carry over to quantum mechanics because the wave function of a particle does not interact with the medium the way an electromagnetic wave does. In particular, in classical quantum theory, unlike in electromagnetic theory, the wave function does not transfer energy to the medium.

The main tenet of our Feynman-type integral description of absorption is that trajectories that propagate into the absorbing surface for the first time are considered to be instantaneously absorbed and are therefore terminated at that surface. The population of the surviving trajectories is therefore discounted by the probability of the absorbed trajectories at each time step.

The process of discounting can be explained as follows. In general, if the trajectories are partitioned into two subsets, the part of the wave function obtained from the Feynman integral over one cannot be used to calculate the probability of this subset, due to interference between the wave functions of the two subsets. However, in the physical situation under consideration, such a calculation may be justified. Our procedure, in effect, assumes a partition of all the possible trajectories at any given time interval $[t, t+\ \Delta t]$ into two classes. One is a class of *bounded trajectories* that have not reached the surface by time $t+\Delta t$ and remain in the domain, and the other is a class of trajectories that hit the surface for the first time in the interval $[t, t+\ \Delta t]$. We assume that the part of the wave function obtained from the Feynman integral over trajectories that hit the surface in this time interval no longer interferes with the part of the wave function obtained from the Feynman integral over the class of bounded trajectories in a significant way. That is, the interference is terminated at this point so that the general population of trajectories can be discounted by the probability of the terminated trajectories. This assumption makes it possible to calculate separately the probability of the absorbed trajectories in the time interval $[t, t+\ \Delta t]$.

The discounting process constitutes a coarse-graining procedure for a large quantum system, describing the absorber. The assumptions we make can be viewed as the mathematical expression of quantum irreversibility of absorption, because the absence of interference separates the two classes of trajectories for all times. Thus the trajectories that stop to interfere can be discounted from the population of trajecotires inside the domain. Our model is only one aspect of irreversible processes.

Under the above assumptions the discounting procedure leads to a Feynman-Kac integral with a killing measure [6], which in turn leads to a Schrödinger equation with zero boundary conditions on the absorbing surface and complex valued energy which depends on the wave function of the class of bounded trajectories at each time t.

We obtain a decay law that is not an exponential rate, in general. It reduces to a rate only for a single energy level initial condition. In this case, the wave function is

a solution of the Schrődinger equation with infinite walls at the absorbing boundaries and constant complex potential that depends on the initial energy. If, however, there are two initial energy levels, the decay law depends on both energy levels and contains an oscillatory term with beat frequency. Similar beats in the decay law occur if the initial wave function contains any number, finite or infinite, of energy levels.

We consider another example, of a Gaussian packet of free particles traveling with a given mean velocity toward an absorbing wall. We find that the packet is partially reflected and partially absorbed and calculate the reflection coefficient. The reflected packet results from trajectories that never reached the wall. This behavior is mainly due to classically forbidden trajectories. In contrast to scattering, this is not the same reflection as that in a finite or infinite barrier, because reflection in a finite barrier depends on the shape of the barrier and reflection in an infinite barrier is totally elastic, whereas the reflection we obtain is discounted by a finite constant factor.

Consider the class $\sigma_{a,b}$ of continuously differentiable functions $x(\tau)$ for $0 \leq \tau < \infty$ such that $a \leq x(\tau) \leq b$ for all $0 \leq \tau < \infty$ and such that $x(0) = x_I,\ x(t) = x$. The class $\sigma_{a,b}$ consists of bounded trajectories that begin at x_I and end at x. We define the Feynman integral over the class $\sigma_{a,b}$ by

$$K(x,t) = \int_{\sigma_{a,b}} \exp\left\{\frac{i}{\hbar} S\left[x(\cdot),t\right]\right\} \mathcal{D}x(\cdot) \tag{1}$$

$$\equiv \lim_{N\to\infty} \alpha^N \int_a^b \cdots \int_a^b \exp\left\{\frac{i}{\hbar} S(x_0,\ldots,x_N,t)\right\} \prod_{j=1}^{N-1} dx_j,$$

where

$$\alpha = \left\{\frac{m}{2\pi i\hbar\Delta t}\right\}^{1/2}.$$

Next, following the method of [7], we show that $K(x,t)$ satisfies Schrödinger's equation and determine the boundary conditions at the endpoints of the interval $[a,b]$. We begin with a derivation of a recursion relation that defines $K(x,t)$. We set

$$K_N(x_N,t) \equiv \alpha^N \int_a^b \cdots \int_a^b \exp\left\{\frac{i}{\hbar} S(x_0,\ldots,x_N,t)\right\} \prod_{j=1}^{N-1} dx_j,$$

then, by definition, $K(x,t) = \lim_{N\to\infty} K_N(x,t)$. We have therefore the recursion relation

$$K_N(x,t) = \alpha \int_a^b \exp\left\{\frac{i}{\hbar}\left[\frac{m(x-x_{N-1})^2}{2\Delta t} - V(x)\Delta t\right]\right\} \times K_{N-1}(x_{N-1},t_{N-1})\,dx_{N-1}. \tag{2}$$

The following derivation is formal, a strict derivation can be constructed along the lines of [7]. We expand the function $K_{N-1}(x_{N-1},t_{N-1})$ in (2) in Taylor's series about x to obtain

$$\begin{aligned} K_N(x,t) = {}& \\ & \alpha e^{-iV(x)\Delta t/\hbar} \int_a^b \exp\left\{\frac{im}{2\hbar\Delta t}(x-x_{N-1})^2\right\} \times \\ & \Bigg[K_{N-1}(x,t_{N-1}) - (x-x_{N-1})\frac{\partial K_{N-1}(x,t_{N-1})}{\partial x} + \\ & \frac{1}{2}(x-x_{N-1})^2 \frac{\partial^2 K_{N-1}(x,t_{N-1})}{\partial x^2} + \\ & O\left((x-x_{N-1})^3\right)\Bigg]\,dx_{N-1}. \end{aligned} \tag{3}$$

We evaluate the integrals in eq.(3) separately for x inside the interval $[a,b]$ and on its boundaries. This leads to the Schrödinger equation

$$i\hbar\frac{\partial K(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 K(x,t)}{\partial x^2} + V(x)K(x,t) \tag{4}$$

for $a < x < b$ with boundary and initial conditions

$$K(a,t) = K(b,t) = 0 \qquad \text{for } t > 0 \tag{5}$$

$$K(x,0) = \delta(x - x_I) \qquad \text{for } a < x < b. \tag{6}$$

Obviously, eqs.(4)-(6) are identical to those of a particle bounded by infinite potential walls.

The same result was obtained in [8] for the case $V(x) = 0$ by a different method. Our method of calculation is essential for calculating the Feynman integral with absorbing boundaries.

First, we calculate the discretized Feynman integral to survive (not to be absorbed) the time interval $[0,\Delta t]$ and to find a trajectory in time Δt at a point x in the interval $[a,b]$. According to the above assumptions, the discretized Feynman integral for trajectories initially inside the interval $[a,b]$ that propagate to the endpoint a for the first time in the time interval $[0,\Delta t]$ is

$$\psi_1(a,\Delta t) = \alpha \int_a^b \Psi_0(x_0) \exp\left\{\frac{i}{\hbar} S(x_0,a,\Delta t)\right\} dx_0.$$

Therefore, the probability density of finding a trajectory at the point a in the time interval $[0,\Delta t]$ is

$$\left|\psi_1(a,\Delta t)\right|^2,$$

and there is an analogous expression for the probability density of finding a trajectory at the point b in the time interval $[0,\Delta t]$. It follows that the probability of a trajectory to be absorbed in the time interval $[0,\Delta t]$ is

$$P_1(\Delta t) = \lambda_a \left|\psi_1(a,\Delta t)\right|^2 + \lambda_b \left|\psi_1(b,\Delta t)\right|^2,$$

where λ_a and λ_b are characteristic lengths (see discussion at the end of the letter). Thus the discretized Feynman

integral to survive the time interval $[0, \Delta t]$ and find a trajectory in time Δt at a point x in the interval $[a, b]$ is

$$\Psi_1(x, \Delta t) = \sqrt{1 - P_1(\Delta t)}\alpha \int_a^b \Psi_0(x_0) \times \exp\left\{\frac{i}{\hbar} S(x_0, x, \Delta t)\right\} dx_0 = \sqrt{1 - P_1(\Delta t)}\, K_1(x, \Delta t). \tag{7}$$

Next, we calculate the discretized Feynman integral to survive the time interval $[\Delta t, 2\Delta t]$ and find a trajectory in time $2\Delta t$ at a point x in the interval $[a, b]$. According to eq.(7), given that a trajectory survived to time Δt, its discretized wave function is $K_1(x, \Delta t)$ so that the discretized Feynman integral to propagate to the point a is

$$\psi_2(a, 2\Delta t) = \alpha \int_a^b K_1(x, \Delta t) \exp\left\{\frac{i}{\hbar} S(x, a, \Delta t)\right\} dx.$$

Proceeding this way, we find that the discretized Feynman integral to survive the time interval $[0, N\Delta t]$ and find a trajectory in time $N\Delta t$ at a point x in the interval $[a, b]$ is

$$\Psi_N(x, N\Delta t) = \sqrt{\prod_{j=1}^{N-1} (1 - P_j(j\Delta t))}\, K_N(x, t), \tag{8}$$

where

$$P_j(j\Delta t) = \lambda_a \left|\psi_j(a, j\Delta t)\right|^2 + \lambda_b \left|\psi_j(b, \Delta t)\right|^2. \tag{9}$$

It remains to calculate the survival probability

$$1 - P(t) = \lim_{N\to\infty} \prod_{j=1}^{N-1} (1 - P_j(j\Delta t)). \tag{10}$$

It can be shown [4] that the probability $P_j(j\Delta t)$ is given by

$$P_j(j\Delta t) = \frac{\hbar \Delta t}{2\pi m}\left[\lambda_a \left|\frac{\partial}{\partial x} K_{j-1}(a, (j-1)\Delta t)\right|^2 + \lambda_b \left|\frac{\partial}{\partial x} K_{j-1}(b, (j-1)\Delta t)\right|^2 + o(1)\right],$$

so that eq.(10) gives

$$1 - P(t) = \tag{11}$$

$$\exp\left\{-\frac{\hbar}{\pi m}\int_0^t \left[\lambda_a \left|\frac{\partial}{\partial x} K(a, t)\right|^2 + \lambda_b \left|\frac{\partial}{\partial x} K(b, t)\right|^2\right] dt.\right\} \tag{12}$$

Now, it follows from eqs.(8) that the wave function of the surviving trajectories at time t is given by

$$\Psi(x, t) = \sqrt{1 - P(t)} K(x, t), \tag{13}$$

and $1 - P(t)$ is given by (11).

Examples

First, we consider a particle with two absorbing walls at $x = \pm a$ and zero potential. We assume that $\lambda_{-a} = \lambda_a$. The wave function is given by

$$K(x, t) = \sum_{n=1}^{\infty} A_n \exp\left\{-\frac{-i\hbar n^2\pi^2}{2ma^2} t\right\} \sin\frac{n\pi}{a} x$$

so that

$$\int_0^t \left|\frac{\partial}{\partial x} K(\pm a, t)\right|^2 dt = \sum_{n=1}^{\infty}\sum_{k\neq n}^{\infty} \frac{A_k \bar{A}_n}{k^2 - n^2} \frac{2knm}{i\hbar a^2} (-1)^{k+n} \times \left[1 - \exp\left\{-\frac{i\hbar\left(k^2 - n^2\right)\pi^2}{2ma^2} t\right\}\right] + \sum_{n=1}^{\infty} |A_n|^2 \frac{n^2\pi^2}{a^2} t.$$

For a particle with a single energy level the wave function decays at an exponential rate proportional to the energy. However, if there are more than just one level, the exponent contains beats. For example, for a two level system with real coefficients, we obtain

$$1 - P(t) = \exp\left\{-\frac{\lambda_a \hbar}{\pi m}\left[\frac{\pi^2}{a^2}\left(A_k^2 k^2 + A_n^2 n^2\right) t - \frac{4mA_k A_n}{\hbar\left(k^2 - n^2\right)} \sin\frac{\hbar\left(k^2 - n^2\right)\pi^2}{2ma^2} t\right]\right\}.$$

The strongest beats occur for $k = 2, n = 1$ with frequency $\omega_{1,2} = \frac{3\hbar\pi^2}{2ma^2}$. Setting $A_1 = A_2 = \sqrt{1/2}$ and introducing the dimensionless time $\tau = \frac{\lambda_a \hbar\pi}{ma^2} t$, we find that

$$1 - P(t) = \exp\left\{-\frac{5}{2}\tau + \frac{2}{3\pi}\sin\frac{3\pi}{2}\tau\right\}. \tag{14}$$

Next, we consider a Gaussian-like wave packet of free particles traveling toward an absorbing wall at $x = 0$ with positive mean velocity k_0. That is, in order to maintain the zero boundary condition on the wall the initial wave function is the difference between two antisymmetric Gaussians relative to the absorbing wall. It follows that

$$\left|\frac{\partial}{\partial x} K(0, t)\right|^2 = \frac{a}{16\pi^2} \frac{\frac{a^4}{16} k_0^2 + x_0^2}{\left(\frac{a^4}{16} + \frac{t^2}{4m^2}\right)^{\frac{3}{2}}} \times \exp\left\{\frac{\frac{a^2}{4}\left(\frac{a^2}{2} k_0^2 + x_0^2\right) - \frac{a^2}{4m} x_0 k_0 t}{\frac{a^4}{16} + \frac{t^2}{4m^2}} - \frac{a^2}{2} k_0^2\right\}, \tag{15}$$

hence

$$\int_0^\infty |\Psi'(0,t)|^2 \, dt < \infty. \tag{16}$$

Thus

$$R = \lim_{t\to\infty} [1 - P(t)] > 0,$$

that is, the wave packet is only partially absorbed. This means that the "reflected" wave consists of trajectories that turned around before propagating into the absorbing wall where absorption occurs. The discount of the wave function occurs when the packet is at the wall, as can be seen from eqs. (15) and (16). Thus R plays the role of a *reflection coefficient.* This is neither the usual reflection coefficient for a finite potential barrier nor that for an infinite barrier.

The two examples can be combined into a simple experimental setup of a cavity with absorbing walls and an absorbing detector at one end. A particle travelling along the axis of the cavity fits the first example in the the transverse direction and the second example in the direction of the cavity axis. Thus the decay law is the product of the two decay laws described above. Further examples and applicatins are discussed in [4].

Discussion

Absorption in a surface is different than absorption in the bulk across the surface in that Feynman trajectories do not propagate across the surface in the former but do in the latter case. This letter is concerned with absorption in a surface. Absorption in the bulk requires a separate theory. The basic assumption in our model is that Feynman trajectories that propagate into the surface are instantaneously absorbed and the probability of the remaining trajectories is discounted by the probability of the absorbed trajectories at each time step. Thus the instantaneous discount factor is proportional to the probability density at the surface at each time step. The proportionality constant, denoted λ, is a characteristic length, in analogy with the scattering length, the mean free path [2], or a typical Compton wavelength. It serves as a fudge parameter in this theory and is expected to be a measurable quantity. It may depend on the energy of the particles, on the temperature of the absorbing medium, and so on.

Our derivation does not start with a Hamiltonian, but rather with an action of bounded trajectories. The resulting decaying wave function corresponds to a classical quantum system with a Hamiltonian whose potential is complex valued and time dependent. This potential depends on the initial energies of the system [12]. Thus, in our formalism, the trajectories are given an actual physical interpretation as the possible trajectories of a quantum particle. This is analogous to the trajectory approach to diffusion in probability theory [5,10,11].

Quantum mechanics without absorption is recovered from our formalism when the absorbing boundaries are moved to infinity. In higher dimensions, quantum mechanics without absorption can be recovered from our formalism by putting absorbing regions with variable density in a half space, say. As the density increases, the boundary of the half space becomes a totally absorbing wall and as the density decreases to zero, quantum mechanics is recovered.

The examples demonstrate the expected phenomenon that particles that reach the absorbing boundary are partially reflected and partially absorbed. In either case the decay pattern of the wave function seems to be new.

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